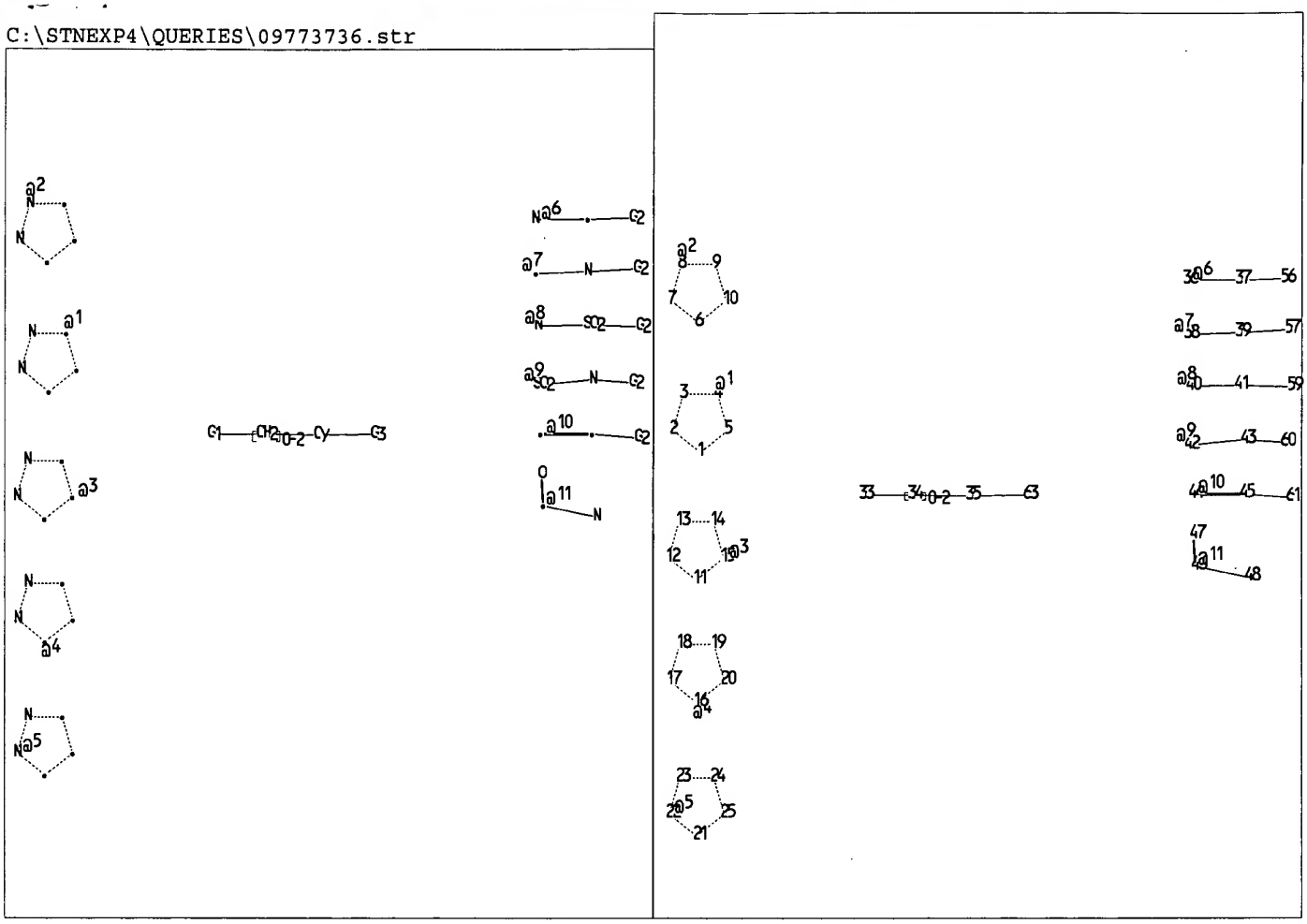
```
=>
Uploading 09773736.str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 07:00:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  16441 TO ITERATE

  6.1% PROCESSED    1000 ITERATIONS                          24 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       321159 TO   336481
PROJECTED ANSWERS:            6700 TO     9082

L2           24 SEA SSS SAM L1
```

Sample search resulted in too many answers.

C:\STNEXP4\QUERIES\09773736.str



chain nodes :
33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 56 57 59 60 61 63
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
48
chain bonds :
33-34 34-35 35-63 36-37 37-56 38-39 39-57 40-41 41-59 42-43 43-60 44-45 45-61
46-47 46-48
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14 14-15
16-17 16-20 17-18 18-19 19-20 21-22 21-25 22-23 23-24 24-25
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14 14-15
16-17 16-20 17-18 18-19 19-20 21-22 21-25 22-23 23-24 24-25 33-34 34-35 35-63
36-37 37-56 38-39 39-57 40-41 41-59 42-43 43-60 45-61 46-47 46-48
exact bonds :
44-45
isolated ring systems :
containing 1 : 6 : 11 : 16 : 21 :

G1:[*1],[*2],[*3],[*4],[*5]

G2:Cy,Ak

G3:[*6],[*7],[*8],[*9],[*10],[*11]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 33:CLASS 34:CLASS 35:Atom 36:CLASS 37:CLASS
38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS
47:CLASS

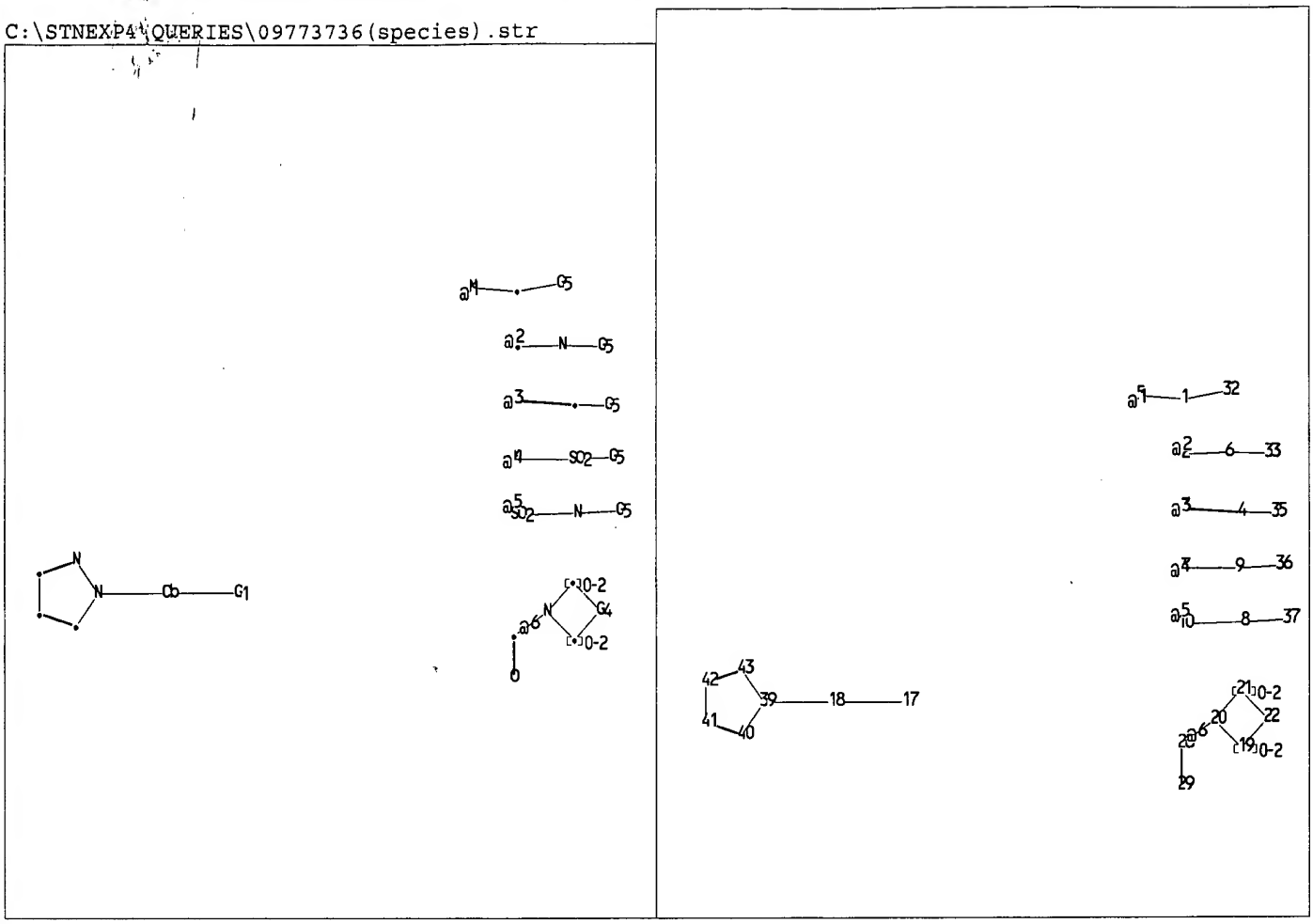
48:Atom 56:CLASS 57:CLASS 59:CLASS 60:CLASS 61:CLASS 63:CLASS

Generic attributes :

35:

Type of Ring System : Monocyclic

C:\STNEXP4\QUERIES\09773736(species).str



chain nodes :
1 2 3 4 5 6 7 8 9 10 17 18 28 29 32 33 35 36 37
ring nodes :
19 20 21 22 39 40 41 42 43
chain bonds :
1-5 1-32 2-6 3-4 4-35 6-33 7-9 8-10 8-37 9-36 17-18 18-39 20-28 28-29
ring bonds :
19-20 19-22 20-21 21-22 39-40 39-43 40-41 41-42 42-43
exact/norm bonds :
1-5 1-32 2-6 3-4 4-35 6-33 7-9 8-10 8-37 9-36 17-18 18-39 19-20 19-22 20-21
20-28 21-22 28-29 39-40 39-43 40-41 41-42 42-43
isolated ring systems :
containing 39 :

G1:[*1],[*2],[*3],[*4],[*5],[*6]

G4:C,O,N

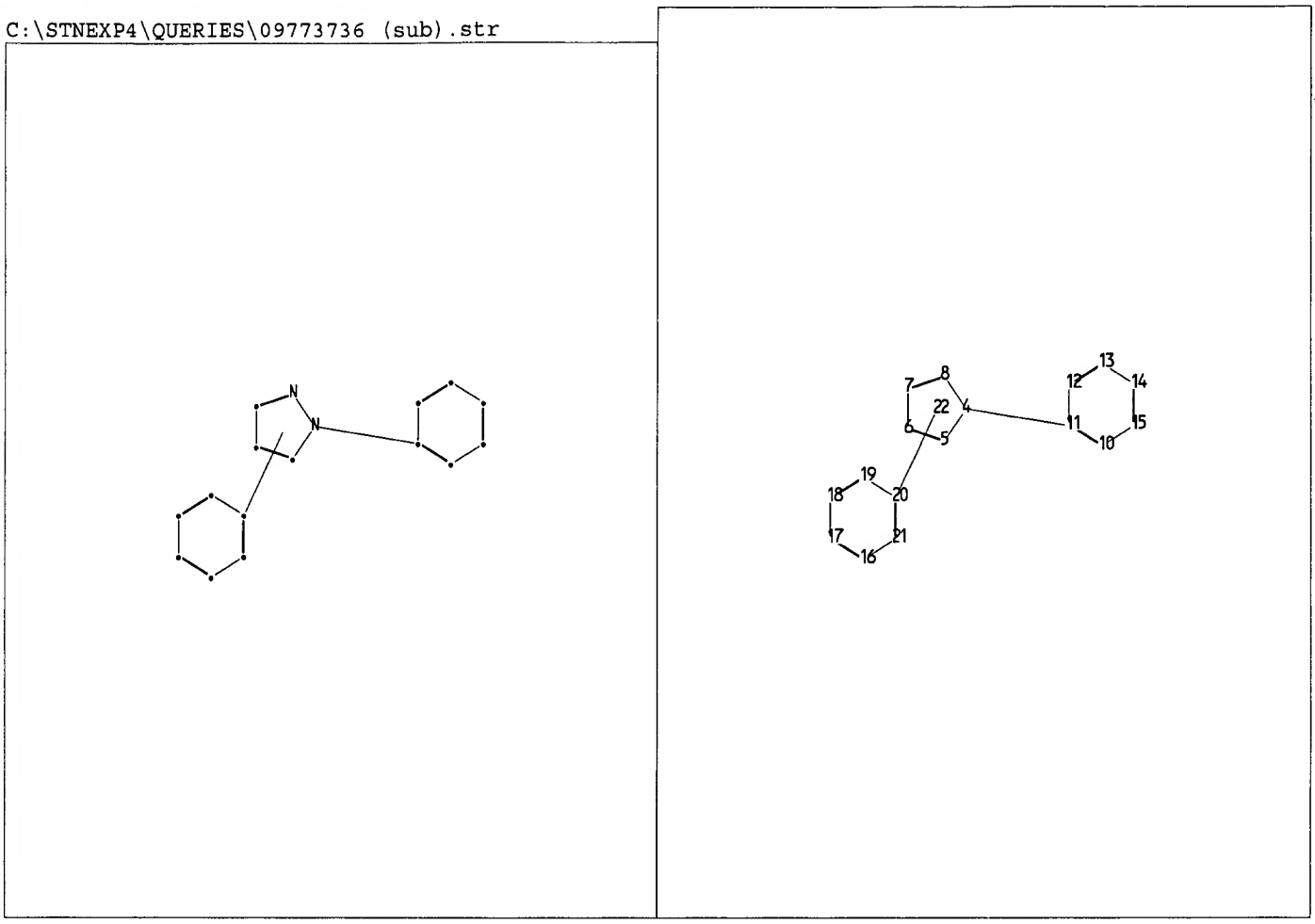
G5:Cy,Ak

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
17:CLASS 18:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 28:CLASS 29:CLASS 32:CLASS
33:CLASS 35:CLASS 36:CLASS 37:CLASS 39:CLASS 40:Atom 41:CLASS 42:CLASS 43:Atom
Generic attributes :
18:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic

Element Count :

Node 18: Limited
C,C6

C:\STNEXP4\QUERIES\09773736 (sub).str



ring nodes :
4 5 6 7 8 10 11 12 13 14 15 16 17 18 19 20 21
chain bonds :
4-11
ring bonds :
4-5 4-8 5-6 6-7 7-8 10-11 10-15 11-12 12-13 13-14 14-15 16-17 16-21 17-18
18-19 19-20 20-21
exact/norm bonds :
4-5 4-8 4-11 7-8
exact bonds :
5-6 6-7
normalized bonds :
10-11 10-15 11-12 12-13 13-14 14-15 16-17 16-21 17-18 18-19 19-20 20-21
isolated ring systems :
containing 4 :

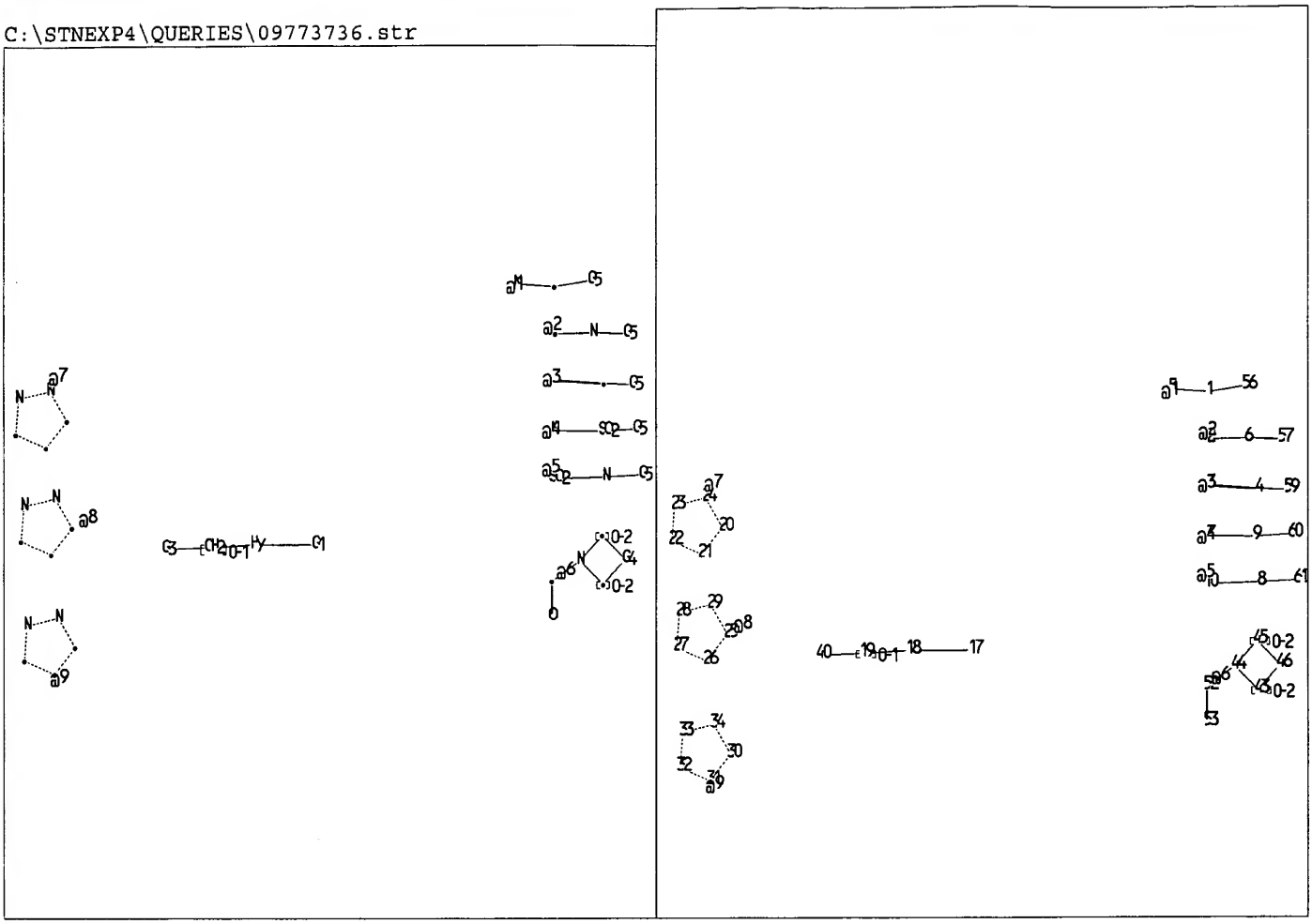
G1

G4:C,O,N

G5:Cy,Ak

Match level :
4:CLASS 5:Atom 6:CLASS 7:CLASS 8:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom
15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS

C:\STNEXP4\QUERIES\09773736.str



chain nodes :
1 2 3 4 5 6 7 8 9 10 17 18 19 40 52 53 56 57 59 60 61
ring nodes :
20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 43 44 45 46
chain bonds :
1-5 1-56 2-6 3-4 4-59 6-57 7-9 8-10 8-61 9-60 17-18 18-19 19-40 44-52 52-53
ring bonds :
20-21 20-24 21-22 22-23 23-24 25-26 25-29 26-27 27-28 28-29 30-31 30-34 31-32
32-33 33-34 43-44 43-46 44-45 45-46
exact/norm bonds :
1-5 1-56 2-6 3-4 4-59 6-57 7-9 8-10 8-61 9-60 17-18 18-19 19-40 20-21 20-24
21-22 22-23 23-24 25-26 25-29 26-27 27-28 28-29 30-31 30-34 31-32 32-33 33-34
43-44 43-46 44-45 44-52 45-46 52-53
isolated ring systems :
containing 20 : 25 : 30 :

G1:[*1],[*2],[*3],[*4],[*5],[*6]

G3:[*7],[*8],[*9]

G4:C,O,N

G5:Cy,Ak

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
17:CLASS 18:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom
27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 40:CLASS 43:Atom
44:Atom 45:Atom 46:Atom 52:CLASS 53:CLASS 56:CLASS 57:CLASS 59:CLASS 60:CLASS
61:CLASS
Generic attributes :

```
    18:
    Saturation              : Unsaturated
    Number of Carbon Atoms  : less than 7
    Type of Ring System     : Monocyclic

Element Count :
    Node 18: Limited
        S,S1
        N,N1
        C,C3
```

```
=>
Uploading 09773736.str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 16:50:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 945871 TO ITERATE

  0.1% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS       0

L2            0 SEA SSS SAM L1

=>
Uploading 09773736.str

L3      STRUCTURE UPLOADED

=> d l3
L3 HAS NO ANSWERS
L3              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l3 sss sam
SAMPLE SEARCH INITIATED 16:54:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  29004 TO ITERATE

  3.4% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:      569932 TO   590228
PROJECTED ANSWERS:              0 TO        0

L4            0 SEA SSS SAM L3
```

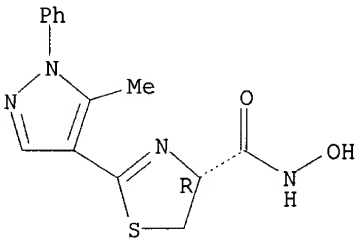
```
=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L5    SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040

L6    SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\09773736.str

L7      STRUCTURE UPLOADED

=> que L7 AND L5 NOT L6

L8   QUE L7 AND L5 NOT L6

=> d l8
L8 HAS NO ANSWERS
L5              SCR 1839
L6              SCR 2016 OR 2026 OR 2039 OR 2040
L7              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L8              QUE  L7 AND L5 NOT L6


=> s l8 sss sam
SAMPLE SEARCH INITIATED 16:55:55 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  24486 TO ITERATE

  4.1% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       480386 TO   499054
PROJECTED ANSWERS:               0 TO        0

L9            0 SEA SSS SAM L7 AND L5 NOT L6

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L10   SCREEN CREATED
```

```
=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047 OR  2046

L11   SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\09773736.str

L12     STRUCTURE UPLOADED

=> que L12 AND L10 NOT L11

L13  QUE L12 AND L10 NOT L11

=> d l13
L13 HAS NO ANSWERS
L10             SCR 1839
L11             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047 OR 2046
L12             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L13             QUE  L12 AND L10 NOT L11


=> s l13 sss sam
SAMPLE SEARCH INITIATED 17:00:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  24486 TO ITERATE

  4.1% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       480386 TO   499054
PROJECTED ANSWERS:               0 TO        0

L14           0 SEA SSS SAM L12 AND L10 NOT L11

=> s l13 sss ful
FULL SEARCH INITIATED 17:01:35 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 488152 TO ITERATE

 81.9% PROCESSED  400000 ITERATIONS                               43 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.12

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       488152 TO   488152
PROJECTED ANSWERS:              43 TO       73

L15          43 SEA SSS FUL L12 AND L10 NOT L11

=> s l15
L16         17 L15
```

=> d l16 1-17 bib,ab,hitstr

L16 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 2002:429779 CAPLUS
DN 137:134487
TI Potent, Novel in Vitro Inhibitors of the Pseudomonas aeruginosa Deacetylase LpxC
AU Kline, Toni; Andersen, Niels H.; Harwood, Eric A.; Bowman, Jason; Malanda, Andre; Endsley, Stephanie; Erwin, Alice L.; Doyle, Michael; Fong, Susan; Harris, Alex L.; Mendelsohn, Brian; Mdluli, Khisimuzi; Raetz, Christian R. H.; Stover, C. Kendall; Witte, Pamela R.; Yabannavar, Asha; Zhu, Shuguang
CS Chiron Corporation, Seattle, WA, 98119, USA
SO Journal of Medicinal Chemistry (2002), 45(14), 3112-3129
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB Deacetylation of uridyldiphospho-3-O-(R-hydroxydecanoyl)-N-acetylglucosamine by LpxC is the first committed step in the Pseudomonas aeruginosa biosynthetic pathway to lipid A; homologous enzymes are found widely among Gram-neg. bacteria. As an essential enzyme for which no inhibitors have yet been reported, the P. aeruginosa LpxC represents a highly attractive target for a novel antibacterial drug. We synthesized several focused small-mol. libraries, each composed of a variable arom. ring, one of four heterocyclic/spacer moieties, and a hydroxamic acid and evaluated the LpxC inhibition of these compds. against purified P. aeruginosa enzyme. To ensure that the in vitro assay would be as physiol. relevant as possible, we synthesized a tritiated form of the specific P. aeruginosa glycolipid substrate and measured directly the enzymically released acetate. Several of our novel compds., predominantly those having fluorinated substituents on the arom. ring and an oxazoline as the heterocyclic moiety, demonstrated in vitro IC50 values less than 1 .mu.M. We now report the synthesis and in vitro evaluation of these P. aeruginosa LpxC inhibitors.
IT **445019-46-5P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(structure activity relationship studies on potent, novel in vitro inhibitors of Pseudomonas aeruginosa deacetylase LpxC)
RN 445019-46-5 CAPLUS
CN 4-Thiazolecarboxamide, 4,5-dihydro-N-hydroxy-2-(5-methyl-1-phenyl-1H-pyrazol-4-yl)-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

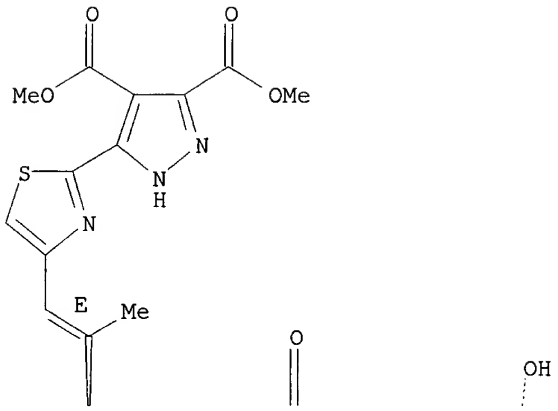
L16 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 2002:240788 CAPLUS
DN 136:263032
TI Preparation of triazolo-epothilones for pharmaceutical use as fungicides and antitumor agents
IN Hoefle, Gerhard; Glaser, Nicole
PA Gesellschaft fuer Biotechnologische Forschung m.b.H. (GBF), Germany
SO PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002024712	A1	20020328	WO 2001-EP10991	20010921
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	DE 10047529	A1	20020411	DE 2000-10047529	20000922
PRAI	DE 2000-10047529	A	20000922		
	DE 2001-10109426	A	20010227		

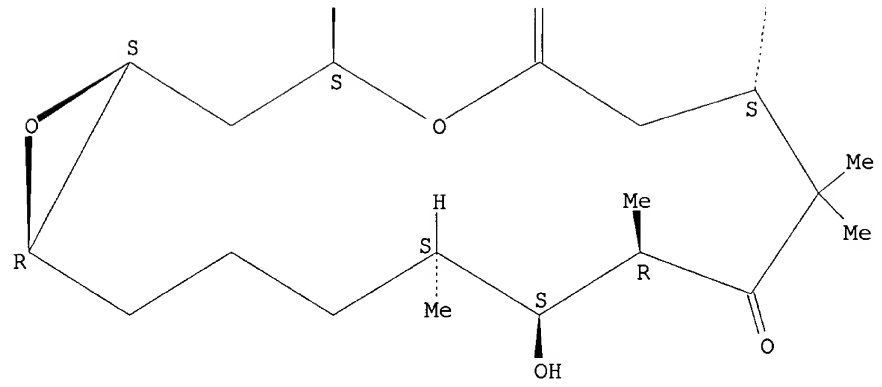
OS CASREACT 136:263032; MARPAT 136:263032
AB Triazolo-thiazole analogs of epothilone A and epothilone B, such as I [R = H, alkyl, aryl, heteroaryl; R1 = H, Me], were prepd. for use as fungicidal and antitumor agents using a 1,3-dipolar cycloaddn. reaction. Thus, epothilone A hydrazone deriv. II was cyclized using NiO2 in CH2Cl2 to give triazolo-thiazole analog I (R = R1 = H) of epothilone A in 49% yield. The prepd. epothilone analogs were tested for activity against L929, K-562, and U-937 human cancer cell lines.
IT **405227-00-1P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of triazolo-epothilones via a 1,3-dipolar cycloaddn. reaction for pharmaceutical use as fungicides)
RN 405227-00-1 CAPLUS
CN 1H-Pyrazole-3,4-dicarboxylic acid, 5-[4-[(1E)-2-[(1S,3S,7S,10R,11S,12S,16R)-7,11-dihydroxy-8,8,10,12-tetramethyl-5,9-dioxo-4,17-dioxabicyclo[14.1.0]heptadec-3-yl]-1-propenyl]-2-thiazolyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A

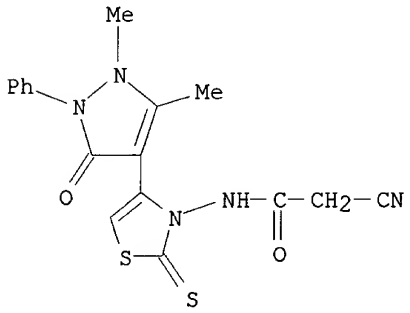


PAGE 2-A

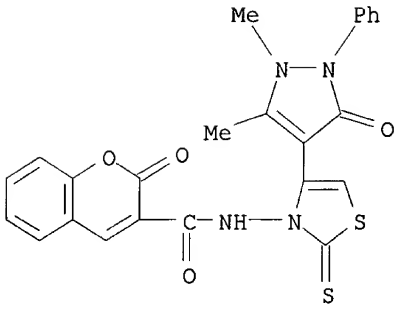


RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 2002:29695 CAPLUS
DN 136:325480
TI Novel synthesis of thiazole, coumarin, pyridine, thiophene and thieno[2,3-b]pyridine derivatives
AU El-Taweel, F. M. A.; Elagamey, A. A.; El-Kenawy, A. A.; Waly, M. A.
CS Department of Chemistry, Faculty of Science, New Damietta, Egypt
SO Phosphorus, Sulfur and Silicon and the Related Elements (2001), 176, 215-225
CODEN: PSSLEC; ISSN: 1042-6507
PB Gordon & Breach Science Publishers
DT Journal
LA English
AB Several new thiazole, coumarin, pyridine, thiophene, and thienopyridines were prepd. from 4-chloroacetylantipyrine and activated nitriles as starting materials.
IT **413570-78-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of thiazole, coumarin, pyridine, thiophene, and thieno[2,3-b]pyridine derivs.)
RN 413570-78-2 CAPLUS
CN Acetamide, 2-cyano-N-[4-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-2-thioxo-3(2H)-thiazolyl]- (9CI) (CA INDEX NAME)

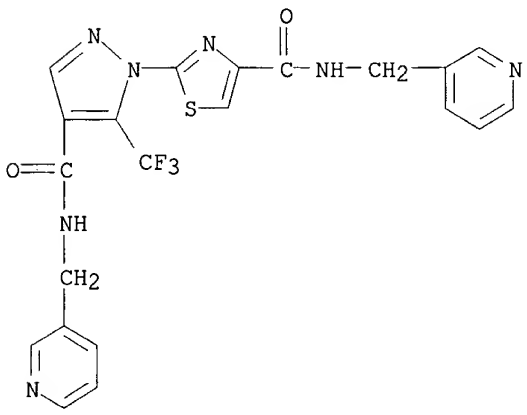


IT **413570-79-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of thiazole, coumarin, pyridine, thiophene, and thieno[2,3-b]pyridine derivs.)
RN 413570-79-3 CAPLUS
CN 2H-1-Benzopyran-3-carboxamide, N-[4-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-2-thioxo-3(2H)-thiazolyl]-2-oxo- (9CI) (CA INDEX NAME)



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 2001:781491 CAPLUS
DN 136:69768
TI Design, Synthesis, and Biological Evaluation of a Library of 1-(2-Thiazolyl)-5-(trifluoromethyl)pyrazole-4-carboxamides
AU Donohue, Bridget A.; Michelotti, Enrique L.; Reader, John C.; Reader, Valerie; Stirling, Matthew; Tice, Colin M.
CS Rohm and Haas Company, Spring House, PA, 19477-0904, USA
SO Journal of Combinatorial Chemistry (2002), 4(1), 23-32
CODEN: JCCHFF; ISSN: 1520-4766
PB American Chemical Society
DT Journal
LA English
AB A library of 422 1-(2-thiazolyl)-5-(trifluoromethyl)pyrazole-4-carboxamides was prepd. in five steps using soln.-phase chem. The first step in the synthesis was the reaction of Et 2-ethoxymethylene-3-oxo-4,4,4-trifluorobutanoate with thiosemicarbazide, which is reported in the literature to afford a 1:1 mixt. of Et 1-thiocarbamoyl-5-(trifluoromethyl)pyrazole-4-carboxylate and Et 1-thiocarbamoyl-3-(trifluoromethyl)pyrazole-4-carboxylate. The product is, however, a single compd., Et 5-hydroxy-1-thiocarbamoyl-5-(trifluoromethyl)-4,5-dihydro-1H-pyrazole-4-carboxylate. This common intermediate was diversified by reaction with 17 .alpha.-bromo ketones affording, in two steps, 17 1-(2-thiazolyl)-5-(trifluoromethyl)pyrazole-4-carboxylic acids. Scavenger resins were used to facilitate formation and purifn. of up to 27 amides from each of these acids in the last step. In addn., the Curtius reaction was applied to 12 of the acids followed by quenching with alcs. to afford a 108-member carbamate library. Certain compds. in the two libraries were toxic to C. elegans.
IT **385416-17-1P**
RL: CPN (Combinatorial preparation); CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and nematocidal activity of a library of 1-(2-thiazolyl)-5-(trifluoromethyl)pyrazole-4-carboxamides and -carbamates)
RN 385416-17-1 CAPLUS
CN 4-Thiazolecarboxamide, N-(3-pyridinylmethyl)-2-[4-[[(3-pyridinylmethyl)amino]carbonyl]-5-(trifluoromethyl)-1H-pyrazol-1-yl]- (9CI) (CA INDEX NAME)



RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 2001:545485 CAPLUS
DN 135:137503
TI Preparation of 3-(phenylheterocyclyl)pyrazole DNA gyrase inhibitors as antibacterial agents
IN Charifson, Paul; Bellon, Steve; Stamos, Dean; Badia, Michael; Grillot, Anne-Laure; Ronkin, Steven; Murcko, Mark; Trudeau, Martin
PA Vertex Pharmaceuticals Incorporated, USA
SO PCT Int. Appl., 110 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001052846	A1	20010726	WO 2001-US1377	20010116

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

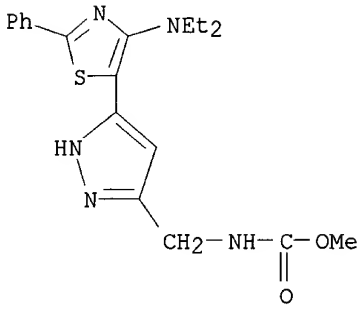
PRAI US 2000-176675P P 20000118
US 2000-254331P P 20001208

AB Disclosed are compds. comprising the pharmacophore features HBA, HBD, Grp1, and at least 2 features selected from Grp2, Grp3, or Grp4 [wherein HBA (H bond acceptor) and HBD (H bond donor) together = (un)substituted pyrazole, 1,2,4-triazole, piperidine, piperazine, thiazole, imidazole, oxazole, etc.; Grp1 = (cyclo)alkyl, (un)substituted carboxy, CONR2, CONHOR, SO2R, SO2NR2, CH2(CH2)nNRCOR, CH2(CH2)nCONR2, CH2(CH2)nSO2NR2, CH:NOR, CH:NNRCOR, CH:NNR2, etc.; Grp2 = H, aliph. group, CONHR, CN, halo, CO2R, SO2R, COR, CONR2, SO2NR2, NRSO2R, NRSO2NR2, Q, COQ, SO2Q, CONHQ, NRSO2Q, or NRSO2NRQ; Grp3 = R, SR, SO2R, SO2NHR, CONHR, CONR2, COR, NHSO2R, NHR, (hetero)aryl, or heterocyclyl; Grp4 = R, SR, SO2R, SO2NHR, CONHR, CONR2, COR, NHSO2R, NHR, halo, (hetero)aryl, or heterocyclyl; R = H or (un)substituted aliph. group; n = 0-1; Q = 3- to 5-membered heterocyclyl or 5- or 6-membered heteroaryl]. The compds. are inhibitors of bacterial DNA gyrase and are useful in treating bacterial infections. For example, condensation of triflic anhydride with 4-hydroxy-2-phenylthiazole-5-carboxylic acid Et ester in the presence of 2,6-lutidine (82%), substitution with piperidine (96%), amidation with N,O-dimethylhydroxylamine.bul.HCl in the presence of Me2AlCl (98%), conversion to the ethanone using MeLi.bul.LiBr (72%), and sequential addn. of KOBu-t, di-Et oxalate, and H2NNH2.bul.H2O gave the 3-(phenylthiazolyl)pyrazole I (59%). Selected compds. of the invention were assayed for ATP hydrolysis activity against E. coli DNA gyrase and exhibited Ki values in the ranges of < 500 nM, 500-1500 nM, and > 1500 nM.

IT **351428-63-2 351428-77-8**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prepn. of heterocyclylpyrazole DNA gyrase inhibitors by conversion of heterocyclylcarboxylic acid methoxy Me amides to ketones and cyclization with hydrazine)

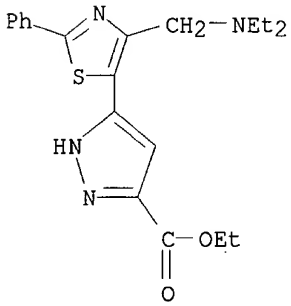
RN 351428-63-2 CAPLUS

CN Carbamic acid, [[5-[4-(diethylamino)-2-phenyl-5-thiazolyl]-1H-pyrazol-3-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 351428-77-8 CAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-[4-[(diethylamino)methyl]-2-phenyl-5-thiazolyl]-, ethyl ester (9CI) (CA INDEX NAME)



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 2001:545484 CAPLUS
DN 135:137502
TI Preparation of 3-(phenylheterocyclyl)pyrazole DNA gyrase inhibitors as antibacterial agents
IN Charifson, Paul; Stamos, Dean; Badia, Michael; Grillot, Anne-laure; Ronkin, Steven; Trudeau, Martin
PA Vertex Pharmaceuticals Inc., USA
SO PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001052845	A1	20010726	WO 2001-US1374	20010116

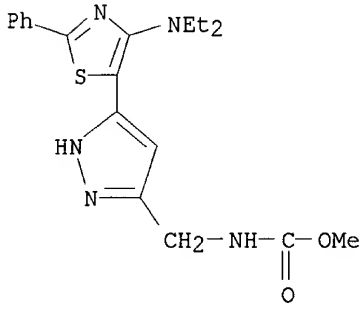
PI W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRAI US 2000-176671P P 20000118
US 2000-254331P P 20001208
OS MARPAT 135:137502
AB Title compds. (I) [wherein A = thiazole, oxazole, (5- to 7-membered fused ring) imidazole, or pyrazole; X = S, O, or NH; Y = C or N; Z = CR3 or NR3; R1 = (un)substituted aliph. group, C(R4)2(CH2)nNRCOR, CR4:NOR, CR4:NOCOR6, CR4:NNRCO2R6, CR4:NNRCOR, CR4:NNR2, C(R4)2(CH2)nNRCO2R6, CO2R6, CONR2, C(R4)2(CH2)nCONR2, C(R4)2(CH2)nSO2NR2, CONHOR, SO2NR2, or C(R4)2(CH2)nNRSO2R6; R2 = H, halo, CN, aliph. group, 3- to 5- membered heterocyclyl, or 5-membered heteroaryl; R3 = (CH2)pN(R5)2 or (un)substituted heterocyclylalkyl, (hetero)aryl, or (hetero)aralkyl; R4 = independently H, (un)substituted aliph. group, or 2 R4 taken together with the C to which they are attached may form a 3- to 6-membered ring; R5 = independently H, (un)substituted aliph. group, or 2 R5 taken together with the N to which they are attached may form a 5- or 6-membered heterocycle; R6 = aliph. group; n = 0-2; p = 0-4; R = independently H or (un)substituted aliph. group; and pharmaceutically acceptable salts thereof] were prepd. I inhibit bacterial gyrase activity and therefore are useful for treating bacterial infections. For example, condensation of triflic anhydride with 4-hydroxy-2-phenylthiazole-5-carboxylic acid Et ester in the presence of 2,6-lutidine (82%), substitution with piperidine (96%), amidation with N,O-dimethylhydroxylamine.bul.HCl in the presence of Me2AlCl (98%), conversion to the ethanone using MeLi.bul.LiBr (72%), and sequential addn. of KOBu-t, di-Et oxalate, and H2NNH2.bul.H2O gave the 3-(phenylthiazolyl)pyrazole II (59%). Selected compds. of the invention were assayed for ATP hydrolysis activity against E. coli DNA gyrase and exhibited Ki values in the ranges of < 500 nM, 500-1500 nM, and > 1500 nM.
IT **351428-63-2P 351428-77-8P 351456-70-7P 351456-72-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heterocyclylpyrazole DNA gyrase inhibitors by conversion of

heterocyclylcarboxylic acid methoxy Me amides to ketones and cyclization with hydrazine)

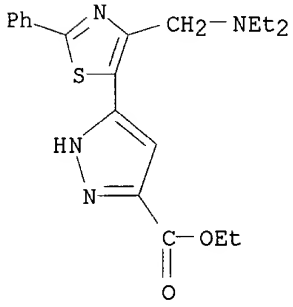
RN 351428-63-2 CAPLUS

CN Carbamic acid, [[5-[4-(diethylamino)-2-phenyl-5-thiazolyl]-1H-pyrazol-3-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)



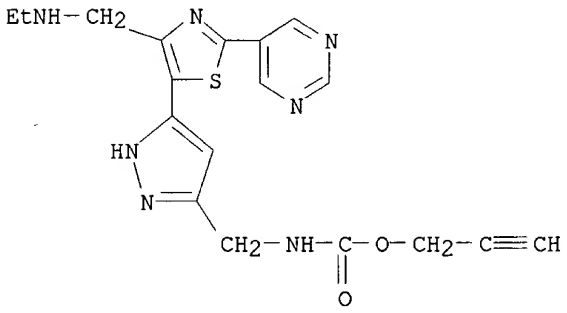
RN 351428-77-8 CAPLUS

CN 1H-Pyrazole-3-carboxylic acid, 5-[4-[(diethylamino)methyl]-2-phenyl-5-thiazolyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 351456-70-7 CAPLUS

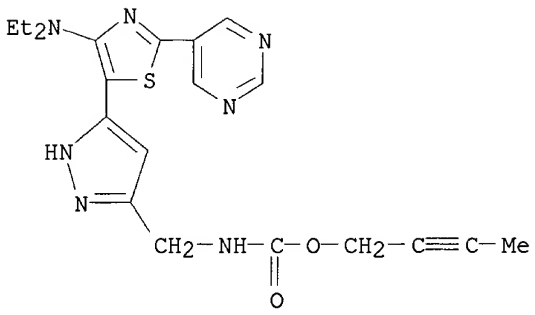
CN Carbamic acid, [[5-[4-[(ethylamino)methyl]-2-(5-pyrimidinyl)-5-thiazolyl]-1H-pyrazol-3-yl]methyl]-, 2-propynyl ester (9CI) (CA INDEX NAME)



RN 351456-72-9 CAPLUS

CN Carbamic acid, [[5-[4-(diethylamino)-2-(5-pyrimidinyl)-5-thiazolyl]-1H-

pyrazol-3-yl]methyl]-, 2-butynyl ester (9CI) (CA INDEX NAME)



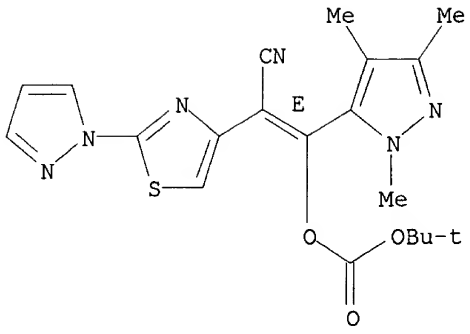
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 2001:228888 CAPLUS
DN 134:266324
TI Preparation of aryl- or heterocyclylacrylonitrile compounds as pest control agents
IN Ogura, Tomoyuki; Murakami, Hiroshi; Numata, Akira; Ueno, Hideki; Kusuoka, Yoshiyuki; Masuzawa, Yoshihide; Miyake, Toshiro; Inoue, Yoichi; Mimori, Norihiko; Takii, Shinji; Itoh, Toshinori
PA Nissan Chemical Industries, Ltd., Japan
SO PCT Int. Appl., 110 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001021618	A1	20010329	WO 2000-JP6324	20000914
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
JP 2001089473	A2	20010403	JP 1999-264453	19990917
PRAI JP 1999-264453	A	19990917		

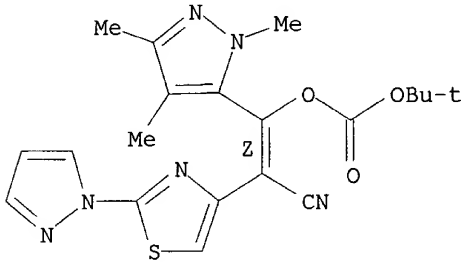
OS MARPAT 134:266324
AB Acrylonitrile compds. represented by formula Q-C(CN):C(A)-OB (wherein Q is thiazolyl substituted by a specific group or pyrazolyl substituted by a specific group; A is Ph optionally substituted by a specific group, naphthyl optionally substituted by a specific group, or a specific heterocyclic group (e.g. thienyl, furyl, pyrrolyl, oxazolyl, isoxazolyl, pyrimidinyl, quinolinyl, etc.) optionally substituted by a specific group; and B is hydrogen, C1-4 alkyl, C1-4 haloalkyl, C2-4 alkoxyalkyl, MeSCH2, MeOCH2CH2OCH2, etc.), which are useful as agricultural chems., esp. pesticides including insecticides, acaricides, aphidicides, and fungicides having low toxicity and low residual property (persistency) and antifouling agents against aquatic organisms, are prepd. Thus, 2.00 g 4-cyanomethyl-2-(2-pyrazinyl)thiazole and 2.44 g 4-chloro-1,3-dimethyl-5-(1-pyrazolylcarbonyl)pyrazole were added to 50 mL THF, treated with 2.22 g potassium tert-butoxide under ice-cooling with stirring, and stirred under ice-cooling for 30 min to give 3-(4-chloro-1,3-dimethylpyrazol-5-yl)-3-hydroxy-2-[2-(2-pyrazinyl)thiazol-4-yl]acrylonitrile (I). I at 500 ppm controlled .gtoreq.80% adult Nephotettix cincticeps on rice leaves.
IT **331714-89-7P 331714-90-0P 331714-91-1P**
331715-10-7P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of aryl- or heterocyclylacrylonitrile compds. as pesticides)
RN 331714-89-7 CAPLUS
CN Carbonic acid, (1E)-2-cyano-2-[2-(1H-pyrazol-1-yl)-4-thiazolyl]-1-(1,3,4-trimethyl-1H-pyrazol-5-yl)ethenyl 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

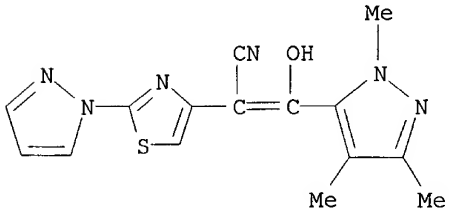


RN 331714-90-0 CAPLUS
CN Carbonic acid, (1Z)-2-cyano-2-[2-(1H-pyrazol-1-yl)-4-thiazolyl]-1-(1,3,4-trimethyl-1H-pyrazol-5-yl)ethenyl 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

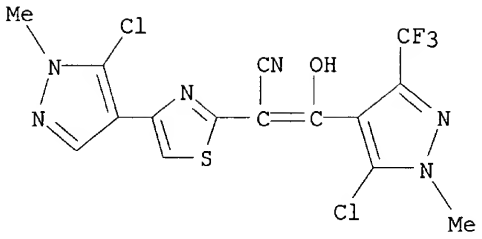
Double bond geometry as shown.



RN 331714-91-1 CAPLUS
CN 4-Thiazoleacetonitrile, .alpha.-[hydroxy(1,3,4-trimethyl-1H-pyrazol-5-yl)methylene]-2-(1H-pyrazol-1-yl)- (9CI) (CA INDEX NAME)

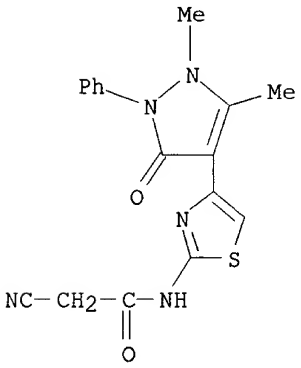


RN 331715-10-7 CAPLUS
CN 2-Thiazoleacetonitrile, 4-(5-chloro-1-methyl-1H-pyrazol-4-yl)-.alpha.-[[5-chloro-1-methyl-3-(trifluoromethyl)-1H-pyrazol-4-yl]hydroxymethylene]- (9CI) (CA INDEX NAME)

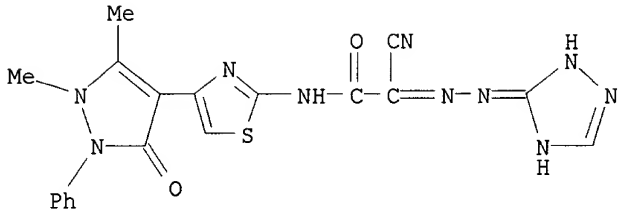


RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

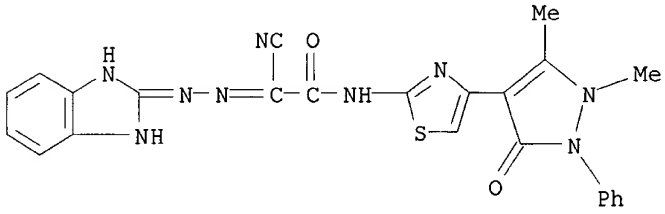
L16 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 2000:523347 CAPLUS
DN 133:266819
TI Polyheterocyclic ring systems with bridgehead nitrogen atoms: a facile route to some novel azolo-1,2,4-triazine derivatives
AU Dawood, Kamal M.; Farag, Ahmad M.; Ragab, Eman A.; Kandeel, Zaghloul E.
CS Department of Chemistry, Faculty of Science, Cairo Univ., Giza, 12613, Egypt
SO Journal of Chemical Research, Synopses (2000), (5), 206-207, 0622-0631
CODEN: JRPSDC; ISSN: 0308-2342
PB Science Reviews Ltd.
DT Journal
LA English
OS CASREACT 133:266819
AB The prepn. of the title azolo-1,2,4-triazines via reaction of functionalized thiazoles with heterocyclic diazonium salts is described. Thus, condensation of the (cyanomethyl)thiazole I with 3-phenyl-1H-pyrazol-5-yl diazonium chloride gave the .alpha.-cyano hydrazone II which cyclized upon heating in pyridine to give the pyrazolotriazine III.
IT **297157-03-0P 297157-09-6P 297157-10-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of bridgehead nitrogen-contg. azolo-triazines via cyclization of heterocyclic hydrazonoacetonitriles)
RN 297157-03-0 CAPLUS
CN Acetamide, 2-cyano-N-[4-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



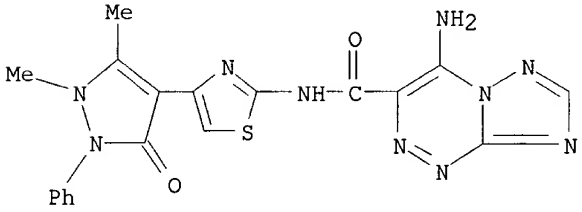
RN 297157-09-6 CAPLUS
CN Acetamide, 2-cyano-N-[4-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-2-thiazolyl]-2-(1H-1,2,4-triazol-3-ylhydrazono)- (9CI) (CA INDEX NAME)



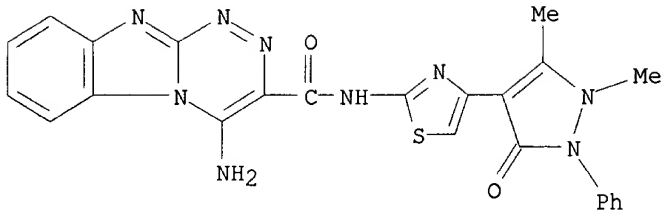
RN 297157-10-9 CAPLUS
CN Acetamide, 2-(1H-benzimidazol-2-ylhydrazono)-2-cyano-N-[4-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-2-thiazolyl]- (9CI) (CA INDEX NAME)



IT **297157-11-0P 297157-12-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of bridgehead nitrogen-contg. azolo-triazines via cyclization of heterocyclic hydrazonoacetonitriles)
RN 297157-11-0 CAPLUS
CN [1,2,4]Triazolo[5,1-c][1,2,4]triazine-3-carboxamide, 4-amino-N-[4-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-2-thiazolyl]- (9CI) (CA INDEX NAME)

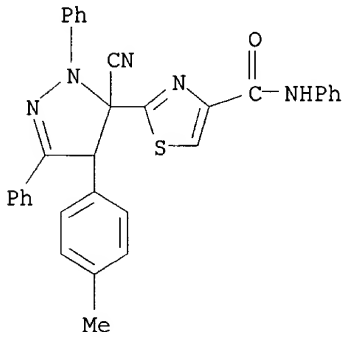


RN 297157-12-1 CAPLUS
CN [1,2,4]Triazino[4,3-a]benzimidazole-3-carboxamide, 4-amino-N-[4-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-2-thiazolyl]- (9CI) (CA INDEX NAME)

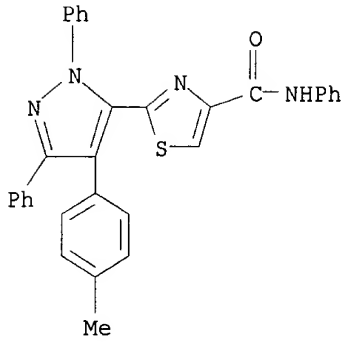


RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 2000:276349 CAPLUS
DN 133:58743
TI Reactions with hydrazonoyl halides. XIX: synthesis of some pyrazole and 5-arylazothiazole derivatives
AU Zohdi, Hussein F.; Rateb, Nora M.; Abdelhamid, Abdou O.
CS Department of Chemistry, Faculty of Science, Cairo University, Giza, Egypt
SO Phosphorus, Sulfur and Silicon and the Related Elements (1998), 133, 103-117
CODEN: PSSLEC; ISSN: 1042-6507
PB Gordon & Breach Science Publishers
DT Journal
LA English
AB Hydrazonoyl chlorides reacted with 2-aryl-1-cyano-1-thiazol-2-ylethenes in the presence of NEt3 to give cycloadducts I (R = Ph, CO2Et, CONHPh; R1 = Ph, 4-MeC6H4; R2 = Ph, 4-Me, 4-ClC6H4, 2-thienyl, 2-furyl) which were converted to the corresponding pyrazoles II by the action of Na methoxide. The reaction of hydrazonoyl halides with each of 2-arylidene-2-cyanoethanethioamides and 2-arylhydrazono-2-cyanoethanethioamides in EtOH-NEt3 or EtOH-NaOH solns. was studied. Structures of all the products were established from their spectral data and alternative synthesis.
IT **277308-40-4P 277308-48-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of pyrazole and 5-arylazothiazole derivs. from hydrazonoyl halides)
RN 277308-40-4 CAPLUS
CN 4-Thiazolecarboxamide, 2-[5-cyano-4,5-dihydro-4-(4-methylphenyl)-1,3-diphenyl-1H-pyrazol-5-yl]-N-phenyl- (9CI) (CA INDEX NAME)



RN 277308-48-2 CAPLUS
CN 4-Thiazolecarboxamide, 2-[4-(4-methylphenyl)-1,3-diphenyl-1H-pyrazol-5-yl]-N-phenyl- (9CI) (CA INDEX NAME)



RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

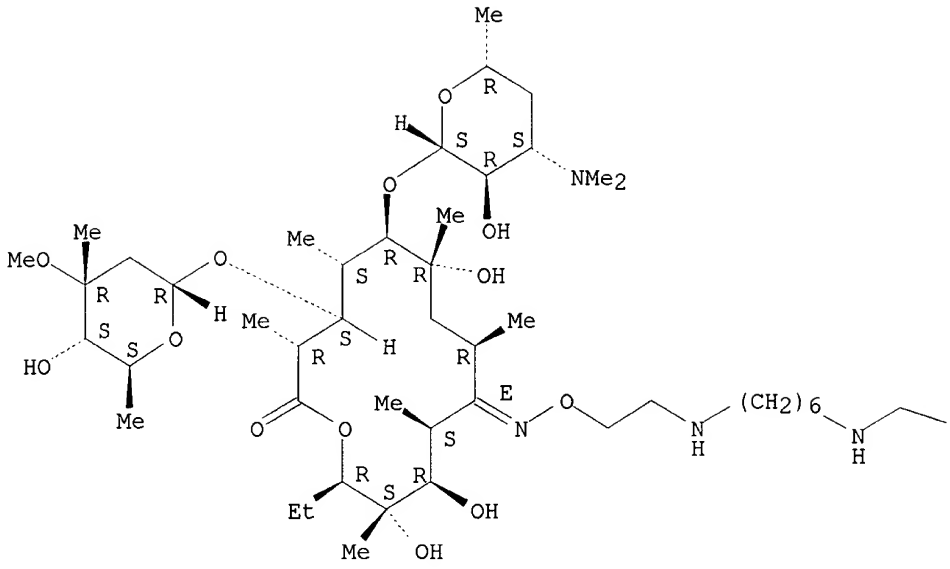
L16 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 2000:98612 CAPLUS
DN 132:122857
TI Preparation of erythromycin derivatives with antibiotic activity
IN Pellacini, Franco; Botta, Daniela; Albini, Enrico; Ungheri, Domenico
PA Zambon Group S.p.A., Italy
SO PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000006606	A2	20000210	WO 1999-EP5485	19990727
	WO 2000006606	A3	20000504		
	W: AU, BR, CA, CZ, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SI, UA, US, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	IT 1301968	B1	20000720	IT 1998-MI1776	19980730
	IT 98MI1776	A1	20000131		
	AU 9952901	A1	20000221	AU 1999-52901	19990727
	EP 1100762	A2	20010523	EP 1999-938386	19990727
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
PRAI	IT 1998-MI1776	A	19980730		
	WO 1999-EP5485	W	19990727		

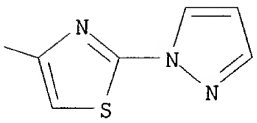
OS MARPAT 132:122857
AB Macrolide erythromycins, e.g. I, were prepd. as antibacterial agents. The invention discloses erythromycin derivs. with antibiotic activity and pharmaceutically acceptable salts thereof, a process for prepg. them and pharmaceutical compns. contg. them as active principle. Erythromycin I (R = R1 = H, Het = R2) was prepd. and tested in vitro against Streptococcus pneumoniae (MIC = 2-4 .mu.g/mL).
IT **256420-52-7P 256420-53-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of erythromycin derivs. with antibiotic activity)
RN 256420-52-7 CAPLUS
CN Erythromycin, 9-[O-[2-[[6-[[[2-(1H-pyrazol-1-yl)-4-thiazolyl]methyl]amino]hexyl]amino]ethyl]oxime], (9E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



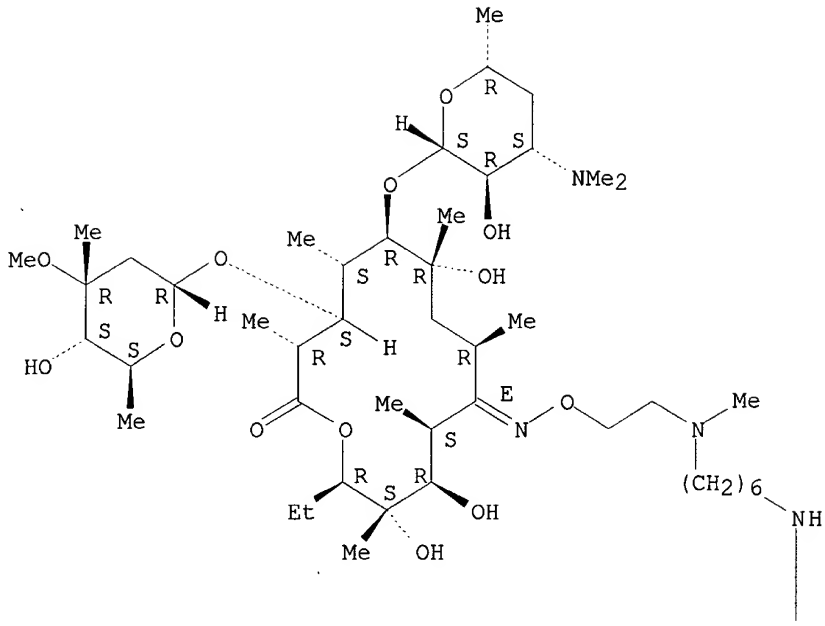
PAGE 1-B



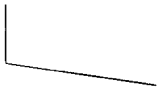
RN 256420-53-8 CAPLUS
CN Erythromycin, 9-[O-[2-[methyl[6-[[[2-(1H-pyrazol-1-yl)-4-thiazolyl]methyl]amino]hexyl]amino]ethyl]oxime], (9E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

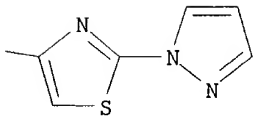
PAGE 1-A



PAGE 2-A



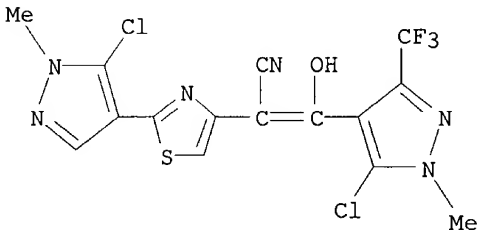
PAGE 2-B



L16 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1999:629944 CAPLUS
DN 131:257583
TI Preparation of heterocyclic compounds having the acrylonitrile moiety as pesticides
IN Ogura, Tomoyuki; Numata, Akira; Ueno, Hideki; Masuzawa, Sadahide; Miyake, Toshio; Inoue, Yoichi; Mimori, Norihiko; Takii, Shinji
PA Nissan Chemical Industries, Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 42 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11269173	A2	19991005	JP 1998-70499	19980319

OS MARPAT 131:257583
AB Title compds. I [Q = thiazolyl or pyrazolyl with substituents; A = (un)substituted Ph, etc.; B = H, alkyl, etc.] are prepd. The title compd. 3-(4-Chloro-1,3-dimethylpyrazol-5-yl)-3-hydroxy-2-(2-pyrazinylthiazol-4-yl)acrylonitrile (prepn. given) at 500 ppm gave .gtoreq. 80% control of Tetranychus urticae.
IT **244772-32-5P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heterocyclic compds. having the acrylonitrile moiety as pesticides)
RN 244772-32-5 CAPLUS
CN 4-Thiazoleacetonitrile, 2-(5-chloro-1-methyl-1H-pyrazol-4-yl)-.alpha.-[[5-chloro-1-methyl-3-(trifluoromethyl)-1H-pyrazol-4-yl]hydroxymethylene]- (9CI) (CA INDEX NAME)



L16 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1999:271338 CAPLUS
DN 130:311815
TI Preparation of pyrazole derivatives as calcium release-dependent calcium channel inhibitors and inhibitors of interleukin-2 (IL-2) production
IN Kubota, Hirokazu; Yonetoku, Yasuhiro; Sugasawa, Keizou; Funatsu, Masashi; Kawazoe, Souichirou; Toyoshima, Akira; Okamoto, Yoshinori; Ishikawa, Jun; Takeuchi, Makoto
PA Yamanouchi Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9919303	A1	19990422	WO 1998-JP4583	19981012
	W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9887139	A1	19990429	AU 1998-87139	19980929
	BR 9803883	A	20000516	BR 1998-3883	19981006
	CA 2304979	AA	19990422	CA 1998-2304979	19981012
	AU 9894593	A1	19990503	AU 1998-94593	19981012
	EP 1024138	A1	20000802	EP 1998-947818	19981012
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	CN 1218046	A	19990602	CN 1998-121354	19981013
	JP 11240832	A2	19990907	JP 1998-290734	19981013
	US 6348480	B1	20020219	US 2000-529131	20000407
	NO 2000001907	A	20000609	NO 2000-1907	20000412
	US 2001011090	A1	20010802	US 2001-773736	20010202
PRAI	JP 1997-279093	A	19971013		
	WO 1998-JP4583	W	19981012		
	US 2000-529131	A3	20000407		

OS MARPAT 130:311815
AB Pyrazole derivs. represented by general formula [I; ring D = pyrazolyl optionally substituted by 1-3 substituents selected from alkyl, lower alkenyl, lower alkynyl, lower haloalkyl, cycloalkylalkyl, alkoxyalkyl, cycloalkyl, alkoxy, CO2H, alkoxycarbonyl, and halo; ring B = phenylene, a nitrogen-contg., divalent, satd. ring group, or an optionally alkylated, monocyclic, divalent heteroarom. ring group; X = -NR1-CR2R3-, -CR2R3-NR1-, -NR1-SO2-, -SO2-NR1- or -CR4:CR5-; wherein R1 = H, OH, alkyl, alkoxy, alkylcarbonyl; R2, R3 = H or alkyl or R2R3 = O or S; R4, R5 = H, halo, lower haloalkyl; A = (1) Ph optionally having one or more substituents, (2) mono-, di- or tricyclic fused heteroaryl optionally having one or more substituents, (3) cycloalkyl optionally having one or more substituents, (4) a nitrogen-contg., satd. ring group optionally having one or more substituents, (5) lower alkenyl optionally having one or more substituents, (6) lower alkynyl optionally having one or more substituents, or (7) alkyl optionally having one or more substituents; or A and X are combined together to represent 1-pyrrolidinylcarbonyl, pyrazolidinylcarbonyl, piperidinocarbonyl, piperazinylcarbonyl, morpholinocarbonyl, 3,4-2H-1,4-benzoxazin-4-ylcarbonyl, or

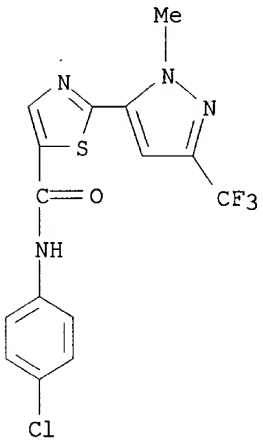
indolylcarbonyl] are prepd. Also claimed are medicinal compns., in particular, calcium release-dependent calcium channel inhibitors, IL-2 prodn. inhibitors, and therapeutics or preventives for allergies, inflammations, or autoimmune diseases, bronchial asthma, or rheumatoid arthritis for contg. the above compds. I as the active ingredients. Thus, 4-methylthiazole-5-carboxylic acid was condensed with 4-[3,5-bis(trifluoromethyl)-1H-pyrazol-1-yl]aniline using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride in 1,2-dichloroethane at room temp. overnight to give the title compd., 4'-pyrazolylthiazole-5-carboxanilide deriv. (II). II in vitro showed IC50 of .ltoreq.1 .mu.M .mu.g/mL for inhibiting the prodn. of IL-2 in Jurkat cells.

IT **223499-67-0P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of pyrazole derivs. as calcium release-dependent calcium channel inhibitors and inhibitors of interleukin-2 prodn. for treatment and prevention of diseases)

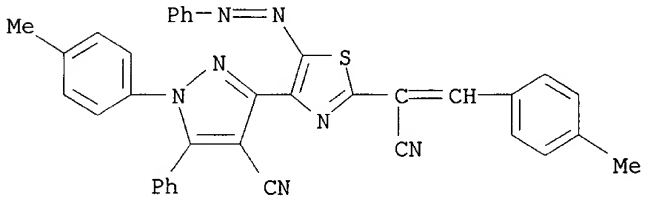
RN 223499-67-0 CAPLUS

CN 5-Thiazolecarboxamide, N-(4-chlorophenyl)-2-[1-methyl-3-(trifluoromethyl)-1H-pyrazol-5-yl]- (9CI) (CA INDEX NAME)

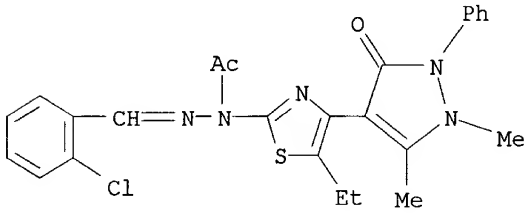


RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

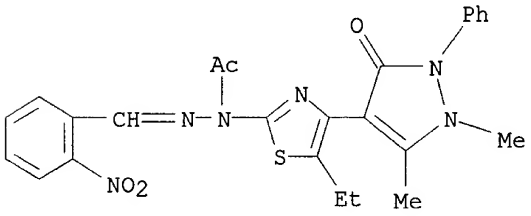
L16 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1996:94723 CAPLUS
DN 124:260989
TI Reactions with hydrazonyl halides. Part 11. Synthesis and reactions of 1-bromo-2-(4-cyano-5-phenyl-1-p-tolypyrazol-3-yl)ethanedione 1-phenylhydrazone
AU Abdelhamid, Abdou O.; Abd-el-Mageid, Fouad F.; Hassan, Nabil M.; Zohdi, Hussein F.
CS Dep. Chem., Cairo Univ., Giza, Egypt
SO Journal of Chemical Research, Synopses (1995), (12), 492-3
CODEN: JRPSDC; ISSN: 0308-2342
PB Royal Society of Chemistry
DT Journal
LA English
AB The reaction of R-CO(Br):NNHPh [R = 4-cyano-1-p-tolyl-5-phenyl-1H-pyrazol-3-yl], with PhSNa, PhSO2Na, thiourea, and KSCN gave hydrazones RCO(SPh):NNPh, a phenylazothiazole I, and a dihydrothiadiazole II, resp. R-CO(Br):NNHPh was also utilized for the synthesis of several heterocycles via its reaction with 2-aminobenzenethiol, 2-aminothiazoles, 2-sulfanylimidazoles, .omega.-phenylsulfonylacetophenone and cyanothioacetamides.
IT **174906-46-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of heterocyclic compds. from cyano(phenyl)pyrazoleethanehydrazonoyl bromide)
RN 174906-46-8 CAPLUS
CN 2-Thiazoleacetonitrile, 4-[4-cyano-1-(4-methylphenyl)-5-phenyl-1H-pyrazol-3-yl]-.alpha.-[(4-methylphenyl)methylene]-5-(phenylazo)- (9CI) (CA INDEX NAME)



L16 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1982:582279 CAPLUS
DN 97:182279
TI Synthesis of some antipyrylthiazolylhydrazones
AU Amal, Hayriye; Ates, Oznur; Salman, Aydin
CS Eczacilik Fak., Univ. Istanbul, Istanbul, Turk.
SO Istanbul Univ. Eczacilik Fak. Mecm. (1980), 16, 96-103
CODEN: IEFMA9; ISSN: 0367-7524
DT Journal
LA English
AB I (R = 3-OMe, R1 = OMe, R2 = H; R = 2-NH2, R1 = R2 = H; R = R2 = H, R1 = NMe2; R = 2-Cl, R1 = H, R2 = Ac) and I (RR1 = 3,4-methylenedioxy, R2 = H) and its hydrobromide were prepd. by reaction of antipyryl .alpha.-bromopropyl ketone with benzaldehyde thiosemicarbazones. Spectral data were given for I.
IT **83539-67-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 83539-67-7 CAPLUS
CN Acetic acid, [(2-chlorophenyl)methylene][4-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-5-ethyl-2-thiazolyl]hydrazide (9CI) (CA INDEX NAME)



L16 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1982:472283 CAPLUS
DN 97:72283
TI Synthesis of some antipyrylthiazolylhydrazones. III
AU Amal, Hayriye; Ates, Oznur; Salman, Aydin
CS Eczacilik Fak., Univ. Istanbul, Istanbul, Turk.
SO Istanbul Univ. Eczacilik Fak. Mecm. (1981), 17, 91-102
CODEN: IEFMA9; ISSN: 0367-7524
DT Journal
LA English
AB Hydrazones I (R = H, R1 = 2-O2NC6H4, 4-O2NC6H4, PhCH:CH; R = Me, R1 = Ph) were obtained in >90% yield by treating the ketone II with RR1C:NNHCSNH2 or RR1CO and H2NNHCSNH2.
IT **82438-80-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 82438-80-0 CAPLUS
CN Acetic acid, 1-[4-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-5-ethyl-2-thiazolyl]-2-[(2-nitrophenyl)methylene]hydrazide (9CI) (CA INDEX NAME)



L16 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1962:2422 CAPLUS
DN 56:2422
OREF 56:477h-i,478a-c
TI Spirobi(m-dioxane) derivatives containing sulfur and halogen
IN Stansbury, Harry A., Jr.; Guest, Howard R.
PA Union Carbide Corp.
DT Patent
LA Unavailable

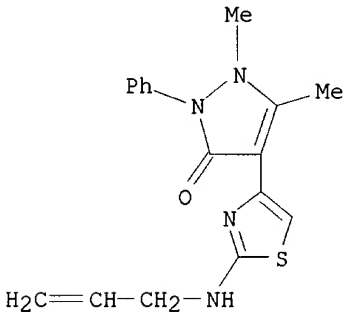
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2992233		19610711	US	

PI US 2992233 19610711 US

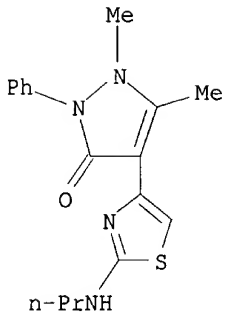
AB A method was described for prepg. S- and halogen-contg. spirobi(m-dioxane) derivs., useful as intermediates and as accelerators for curing rubber, by treating a 3,9-divinylspiro(m-dioxane) deriv. with ZSmX, where X = Cl, Br, or iodine, m = 1 or 2, and Z = lower alkyl, haloalkyl, alicyclic, aryl, alkaryl, aralkyl, Cl (when X = Cl) and Br (when X = Br and m = 2). 3,9-Divinylspirobi(m-dioxane) (I) (42 g.) in 84 g. C6H6 stirred at 25.degree. while adding 45 g. SCl2 during 30 min., the mixt. refluxed, the volatiles removed at 58.degree./10 mm., the residue (84 g.) dissolved in 400 ml. hot Me2CO, and the soln. dild. with 700 ml. MeOH gave 40 g. II, m. 162-80.degree.. From I and S2Cl2 was similarly prepd. III, m. 75-83.degree.. I (106 g.) and 215 g. 95% Cl3CSCl heated 2 hrs. at 140.degree. gave 191 g. IV, liquid, n30D 1.5381.

IT **93650-32-9**, Antipyrine, 4-[2-(allylamino)-4-thiazolyl]-
93726-20-6, Antipyrine, 4-[2-(propylamino)-4-thiazolyl]-
95136-28-0, Antipyrine, 4-[2-(phenethylamino)-4-thiazolyl]-
97737-92-3, Antipyrine, 4-[2-(propylamino)-4-thiazolyl]-, hydrochloride **98340-33-1**, Antipyrine, 4-[2-(allylamino)-4-thiazolyl]-, hydrochloride
(prepn. of)

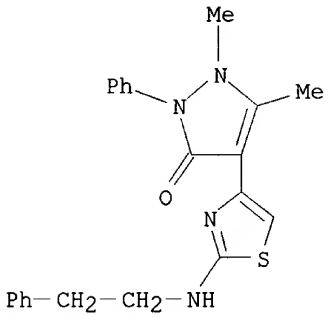
RN 93650-32-9 CAPLUS
CN Antipyrine, 4-[2-(allylamino)-4-thiazolyl]- (7CI) (CA INDEX NAME)



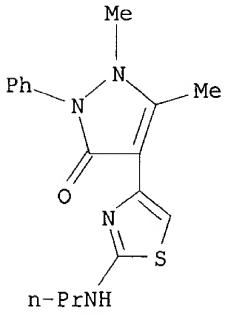
RN 93726-20-6 CAPLUS
CN Antipyrine, 4-[2-(propylamino)-4-thiazolyl]- (7CI) (CA INDEX NAME)



RN 95136-28-0 CAPLUS
CN Antipyrine, 4-[2-(phenethylamino)-4-thiazolyl]- (7CI) (CA INDEX NAME)

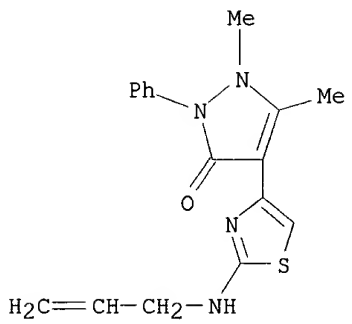


RN 97737-92-3 CAPLUS
CN Antipyrine, 4-[2-(propylamino)-4-thiazolyl]-, hydrochloride (7CI) (CA INDEX NAME)



● x HCl

RN 98340-33-1 CAPLUS
CN Antipyrine, 4-[2-(allylamino)-4-thiazolyl]-, hydrochloride (7CI) (CA INDEX NAME)



●x HCl

L16 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2002 ACS
AN 1962:2421 CAPLUS
DN 56:2421
OREF 56:477f-h
TI Pyrazolone derivatives
IN Stenzl, Johann; Halfliger, Franz
PA Geigy Chemical Corp.
DT Patent
LA Unavailable

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2993052		19610718	US	

AB XC:CH.S.C(NHR):N (X = antipyrinyl throughout) (I) were prepd., wherein R is a lower alkyl or alkenyl radical, Ph, or a phenylalkyl radical, by treating XCOCH2Z (II) (Z = Cl or Br) with a monosubstituted thiourea, H2NCSNHR (III). II (Z = Cl) (m. 167.degree.) [Kaufmann, et al., CA 37, 47321] 27 and III (R = Me) 10 in EtOH 200 parts refluxed 6 hrs., cooled, dild. with H2O 1000, and made alk. with aq. NH3 gave I (R = Me), m. 176-8.degree.; HCl salt m. 208-10.degree. (decompn.). Similarly, II (Z = Br) (m. 148-9.degree.) [prepd. by brominating II (Z = H) in AcOH while irradiating with an ultraviolet lamp] 25 and III (R = Et) 10 in EtOH 100 parts refluxed 3 hrs. gave I (R = Et), m. 163-5.degree.; HCl salt m. 208-11.degree. (decompn.). Similarly were prepd. the following I (R, m.p., and m.p. of HCl salt given): Pr, 170-1.degree. (EtOH), 187-90.degree. (decompn.); allyl, 172-3.degree. (EtOH), 171-4.degree. (decompn.); PhCH2CH2, 145-6.degree. (EtOH),-; Ph, 243-5.degree. (EtOH), 102-6.degree. (decompn.). The I have antiphlogistic and analgesic activity.

IT **93022-47-0**, Antipyrine, 4-[2-(ethylamino)-4-thiazolyl]-
93650-32-9, Antipyrine, 4-[2-(allylamino)-4-thiazolyl]-
93726-20-6, Antipyrine, 4-[2-(propylamino)-4-thiazolyl]-
95136-28-0, Antipyrine, 4-[2-(phenethylamino)-4-thiazolyl]-
97737-92-3, Antipyrine, 4-[2-(propylamino)-4-thiazolyl]-, hydrochloride **98111-64-9**, Antipyrine, 4-[2-(ethylamino)-4-thiazolyl]-, hydrochloride **98340-33-1**, Antipyrine, 4-[2-(allylamino)-4-thiazolyl]-, hydrochloride
(prepn. of)

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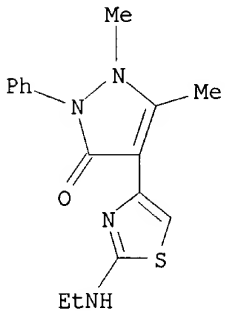

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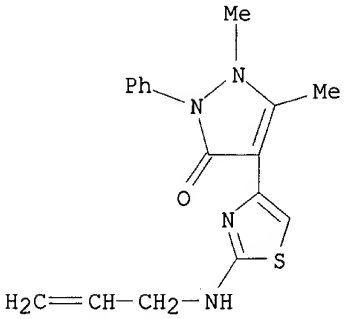

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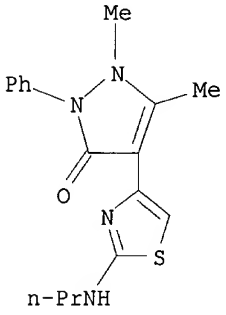

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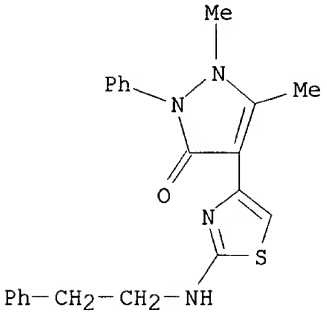

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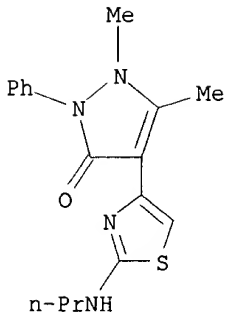

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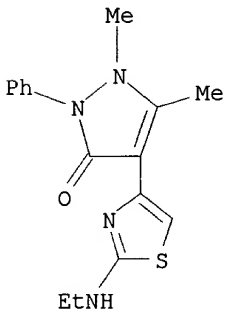

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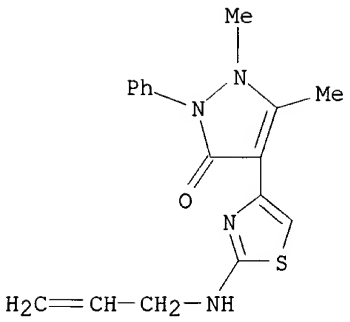

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L7             STRUCTURE UPLOADED
L8             QUE L7 AND L5 NOT L6
L9           0 S L8 SSS SAM

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L12            STRUCTURE UPLOADED
L13            QUE L12 AND L10 NOT L11
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L17          2 L15

=> d l17 1-2 bib,hitstr
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L17 ANSWER 1 OF 2 CAOLD COPYRIGHT 2002 ACS
AN CA56:477h CAOLD
TI spiro(m-dioxane) derivs. contg. S and halogen
AU Stansbury, Harry A., Jr.; Guest, H. R.
DT Patent
TI spirobi-m-dioxane derivs. contg. S and halogen
PA Union Carbide Corp.
DT Patent

PATENT NO.	KIND	DATE
US 2992233		1961

IT **93650-32-9 93726-20-6 95136-28-0**
97737-92-3 98340-33-1
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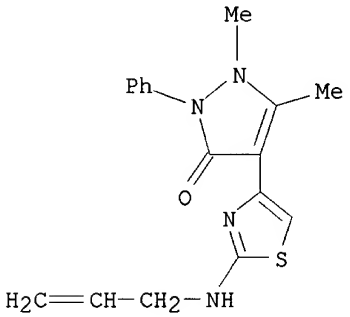

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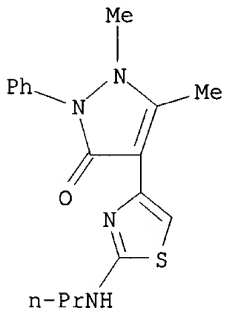

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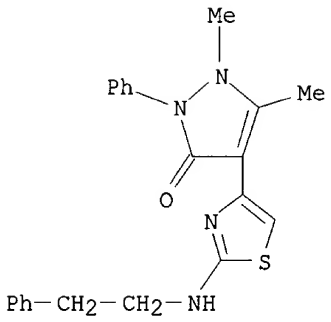

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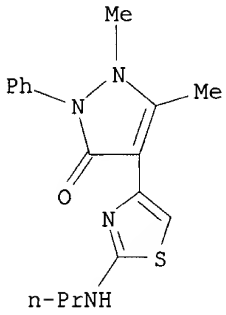

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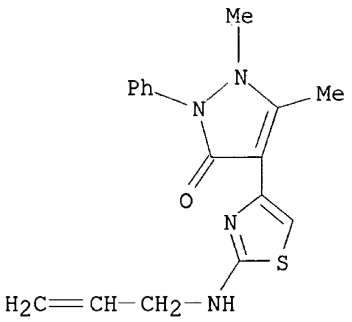

●x HCl

L17 ANSWER 2 OF 2 CAOLD COPYRIGHT 2002 ACS
AN CA56:477f CAOLD
TI pyrazolone derivs.
AU Stenzl, Johann; Haefliger, F.
PA Geigy Chemical Corp.
DT Patent

PATENT NO.	KIND	DATE
US 2993052		1961

IT **93022-47-0 98111-64-9**
RN 93022-47-0 CAOLD
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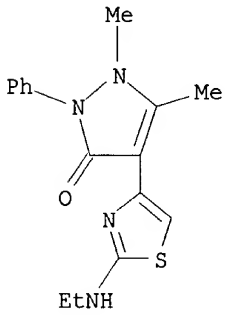

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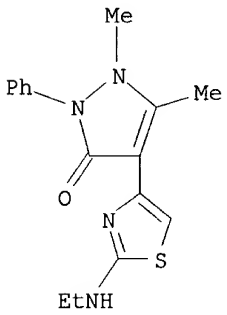

●x HCl

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
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